A surface resolution criterion for two-phase flows DNS

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Abstract

Two-phase flows occur in many fields such as liquid fuel injection, plunging waves, cavitation, sloshing, spray, phase change, pipeline of two-phase flows, etc. Regarding numerical developments, a lot of improvements have been realised to describe the interface between liquid and gas. Especially, the objective of Direct Numerical Simulations (DNS) is to solve all the scales of the considered flow. However, unlike the Kolmogorov scale in single phase flows, no theory about the smallest scale in a two-phase turbulent flow has been developed yet. Indeed, the liquid structures that break up, become smaller and smaller and make such theoretical work difficult. Two main scales are expected to have a strong influence in a two-phase system: one emerging from small scale turbulence-interface interactions and another linked to the smallest scale of wrinkling of the surface. The aim of this study is to investigate the latter and to provide a criterion to evaluate the interface resolution quality (IRQ) based on surface geometry. IRQ criteria have already been proposed in previous works with one based on the surface density used in ELSA (Eulerian Lagrangian Spray Atomization) approach or another one based on liquid volume fraction gradient. These criteria are not well adapted for DNS with interface capturing method coupled with a reconstruction technique. Consequently, an IRQ criterion based on curvature is here proposed to evaluate the accuracy of the interface resolution. The ARCHER code is used to simulate an Homogeneous Isotropic Turbulent (HIT) configuration to perform a mesh convergence study to evaluate the effect of various resolutions on important statistics (surface density, mean IRQ). Then, a diesel jet case (based on ECN Spray A) is presented to show the level of accuracy and pertinence of the IRQ criterion on this kind of configuration.

Keywords

Resolution criterion ; DNS ; interface ; two-phase flows ; IRQ.

Introduction

Since the first studies on atomization DNS [1, 2, 3], the question of the required resolution to assess that a simulation is a "true DNS" is still unanswered. As mentioned in Gorokhovski and Herrmann [4], few DNS studies illustrate their grid dependency with a grid convergence analysis. A discussion on the smallest scale observable in a two-phase flow DNS is also present, arguing that reaching a true two-phase DNS resolution is more expensive than its single-phase counterpart, due to breakup events leading to liquid structures becoming smaller and smaller. Later, Shinjo and Umemura [5] performed a computation with 6 billion points and despite this important effort in terms of mesh resolution (3 different grids studied), it is not clear that the smallest scale has been captured with the finest mesh. However, the minimum size of structures encountered in a two-phase system should be governed by an equilibrium between turbulence and surface tension. In a sense, it should be possible to define a criterion describing turbulence-interface interactions and the smallest scale emerging from these interactions, and another focusing on the resolution of the interface topology, based on the interface curvature. The first one is of utmost importance, but there are still no studies in the literature that demonstrate theoretically the smallest scale of a dense turbulent two-phase flow system, such as the Kolmogorov scale in single-phase flow. The second one is easier to understand, and is the subject of this work. Indeed, one can argue that the smallest scale of wrinkling is directly related to the interface curvature. When the curvature is too strong, the interface capturing/tracking method fails to represent the topological change and this failure can have a local or global impact on the atomization mechanism. To identify this kind of issue, a definition of a criterion called Interface Resolution Quality (IRQ) is proposed in this work. Note that a similar criterion has been developed in the context of atomization modeling [6] to switch from an interface capturing method (used in well-resolved regions), to a turbulent two-phase mixing model called ELSA [7, 8] in under-resolved regions. To illustrate the potential of this criterion, two main configurations have been considered, using the well-known ARCHER code [9, 10, 3, 11]: a liquid jet corresponding to the Spray A from the ECN (Engine Combustion Network) and a two-phase Homogeneous Isotropic Turbulence (HIT). Concerning the Spray A, it is evident that the real Weber and Reynolds numbers are too high to be described by DNS. However, it is a good candidate to observe the behavior of the IRQ criterion in an under-resolved scenario. Then, the Weber and Reynolds numbers are dumped to reach the usual order of magnitude encountered in most liquid jet DNS studies, which correspond to a well-resolved scenario.

Governing equations and numerical methods

Here, a joint Level Set/VOF method is coupled with a projection method to carry out the direct numerical simulation of incompressible Navier-Stokes equations:

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \vec{\nabla} \vec{u} = -\frac{\vec{\nabla} P}{\rho} + \frac{1}{\rho} \vec{\nabla} \cdot (2\mu D) + \vec{f} + \frac{1}{\rho} \sigma \kappa \delta (\varphi) \vec{n} \quad (1)$$

where P is the fluid pressure, $\vec{u}$ is the velocity vector, and D is the viscous deformation tensor. At the interface, the surface tension force can be considered based on the Dirac function $\delta(\varphi)$. Concerning the interface capturing method, a CLSVOF (Coupled Level Set Volume Of Fluid) interface capturing method is used to ensure mass conservation and an accurate description of the interface topology (See [3] for details).

This work benefits for the latest improvements of the ARCHER code: the convective term is solved using the improved Rudman technique presented in Vaudor et al. [11], allowing a better accuracy and description of high density ratio flows. This method is based on the computation of mass fluxes from the Volume Of Fluid (VOF) method, which can then be used in a conservative formalism of the convective term. The diffusive term is now computed with the approach of Sussman et al. [12], the main advantage of this method is the implicit jump condition of the viscous tensor.

Fluid dynamics equations are solved in the context of a low Mach number approach, based on a projection method for the direct numerical simulation of incompressible Navier-Stokes equations (detailed in Vaudor et al. [11]). The viscosity depends on the sign of the level set function according to each phase (liquid and gas). To finalize the description of the two-phase flow, jump conditions across the interface are taken into account with the ghost fluid (GF) method. In the GF method, ghost cells are defined on each side of the interface ([13, 14]). This prolongs each phase to allow smooth derivatives in the vicinity of the interface. As defined previously, the interface is characterized through the distance function, and jump conditions are extrapolated on a few nodes on each side of the interface.

The computation of the curvature is the same as in Canu et al. [9] and is based on the distance function (φ) that is part of the numerical procedure in the resolution of the two-phase flow Navier-Stokes equations. A more detailed explanation of such method is available in Kindlmann et al. [15].

Interface Resolution Quality definition

The Interface Resolution Quality IRQ_κ is directly dependent of the local principal curvatures (κ_1, κ_2) and the mesh size Δx:

$$IRQ_\kappa = \frac{1}{\Delta x |\kappa_1 + \kappa_2|} \quad (2)$$

This criterion highlights under-resolved regions of the interface and when averaged gives an indication of the quality of the total simulation. For instance, an IRQ equal to 1 is equivalent to two mesh cells in the radius of a sphere, and consequently presents a poorly-resolved area. On the contrary, an IRQ greater than 2 indicates well resolved area and, in the case of a sphere, corresponds to a radius with four mesh cells. The chosen value of 2 for resolved areas represents the minimum for an accurate simulation. Besides, there is no definition of the smallest scales in two-phase flows and only a mesh convergence study can be done to ensure that the flow is fully resolved. Indeed, the smallest scales of interface in events like breakups tend toward 0 and can never be captured. Despite the fact that simulations are not able to capture these smallest scales of interface, they can be refined sufficiently to capture the specified features and main statistics of the flow. Therefore, the preservation of these features and statistics can define a well resolved interface.

Results and discussion

The first case to be validated is a Homogeneous Isotropic Turbulent box (HIT) with periodic boundary conditions. The turbulence is represented by a forcing term like the one used in previous works [16, 17, 10, 18], in order to impose a turbulent kinetic energy $\bar{k}_{kin} = 3.6\ m^2 \cdot s^{-2}$. The physical parameters are presented in Table 1.

Table 1. Physical parameters for the HIT box.

ρ_g $(kg \cdot m^{-3})$	ρ_l $(kg \cdot m^{-3})$	μ_g $(kg \cdot m^{-1} \cdot s^{-1})$	μ_l $(kg \cdot m^{-1} \cdot s^{-1})$	σ $N \cdot m^{-1}$
25	753	1.879×10^{-5}	5.65×10^{-4}	0.0135

The domain is a cube with $L = 1.5 \times 10^{-4}\ m$ and is enmeshed with a $256 \times 256 \times 256$ grid. A case with $\phi = 5\%$ of liquid is presented here.

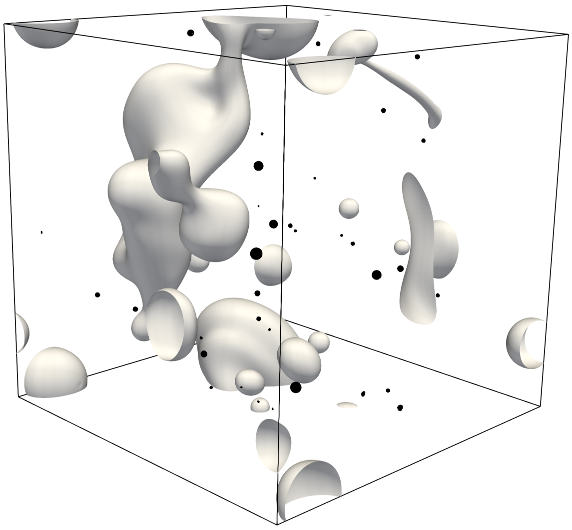

Figure 1. Surface representation of the HIT 5%. In black, surfaces with an IRQ less than 2.

This case is supposed to be a well-defined case based on previous works. As we can see in Figure 1, only few number of droplets are colored in black which correspond to poorly-resolved surfaces. These surfaces colored in black have an IRQ less than 1 which mean that the droplets' radius is less than $2\Delta x$. The curvature in these regions is too strong to be well captured. The percentage of under-resolved surface is low: around 1% for an IRQ less than 1 and around 3% for an IRQ less than 2, illustrating well-resolved case. Besides, the converged value of the mean surface density Σ is plotted on Figure 2 for 32^3, 64^3, 128^3, 192^3 and 256^3 meshes. A convergence is observed from the 128^3 mesh point, indicating, again, a well-resolved case for a 256^3 mesh.

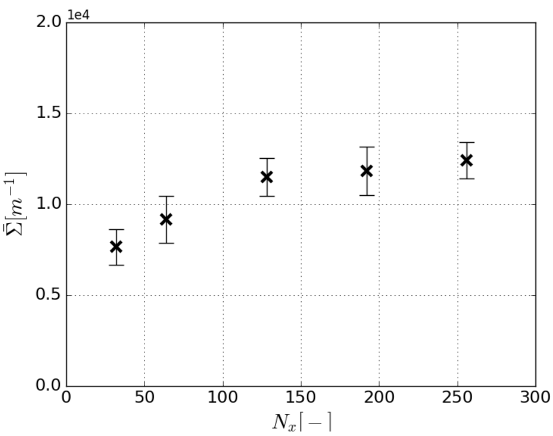

Figure 2. Mesh convergence of the mean surface density Σ for the HIT 5%. The error bars correspond to the standard deviation of the surface density value.

The second case to be validated is a diesel jet based on the ECN Spray A configuration [19]. The domain measures $445 \times 445 \times 1780\ \mu m^3$ and the simulation is performed on a $256 \times 256 \times 1024$ grid. The injector has a diameter $D_{inj} = 89.4\ \mu m$. For the inlet boundary condition, the velocities are extracted from the outlet plane of a LES simulation inside the injector based on the study of Anez et al. [6]. All the other boundaries are outflow boundary conditions. The physical parameters are shown in Table 2.

Table 2. Physical parameters for the ECN Spray A configuration.

ρ_g $(kg \cdot m^{-3})$	ρ_l $(kg \cdot m^{-3})$	μ_g $(kg \cdot m^{-1} \cdot s^{-1})$	μ_l $(kg \cdot m^{-1} \cdot s^{-1})$	σ $N \cdot m^{-1}$
22.8	713	1.8343×10^{-5}	7.248×10^{-4}	0.0243

This corresponds to the original Spray A case with high Weber ($We \simeq 1044$) and Reynolds ($Re \simeq 70356$) numbers. The relations used for these numbers are:

$$We = \frac{\rho_g u_{max}^2 D_g}{\sigma} \quad (3)$$

$$Re = \frac{\rho_l u_{max} D_{inj}}{\mu_l} \quad (4)$$

with $D_g = \Delta x$ like in Menard et al. [3]. This case can't be described accurately in DNS due to these high numbers but it can be interesting to see the accuracy with original parameters. An other Spray A case has been performed with lower Weber ($We \simeq 10$) and Reynolds ($Re \simeq 5795$) numbers like in Menard et al. [3] in order to have a better resolution. The new parameters are in Table 3.

Table 3. Physical parameters for the modified ECN Spray A configuration (low Weber and Reynolds numbers).

ρ_g $(kg \cdot m^{-3})$	ρ_l $(kg \cdot m^{-3})$	μ_g $(kg \cdot m^{-1} \cdot s^{-1})$	μ_l $(kg \cdot m^{-1} \cdot s^{-1})$	σ $N \cdot m^{-1}$
22.8	713	1.8343×10^{-5}	8.8×10^{-3}	2.54

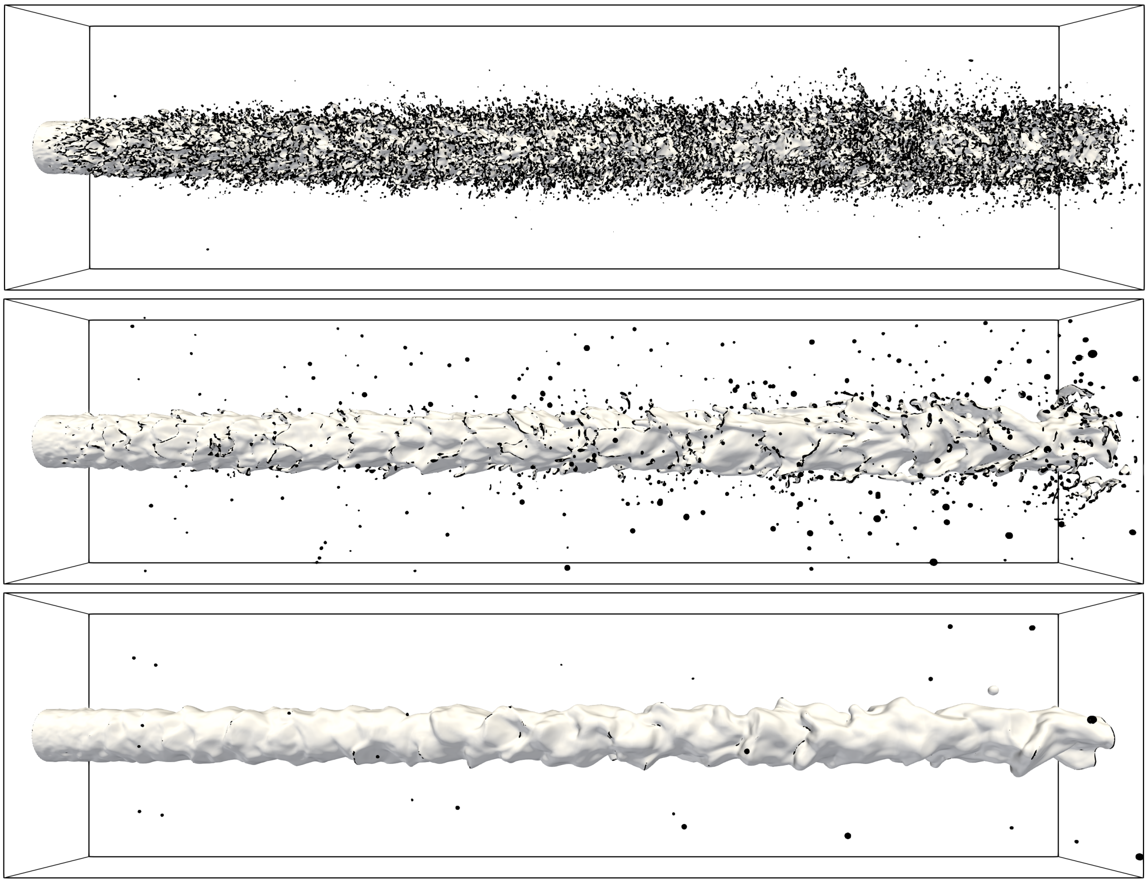

Figure 3. Surface representation of the Spray A configuration for high Weber and Reynolds numbers ($We \simeq 1044$ and $Re \simeq 70356$) (top), low Weber and Reynolds numbers ($We \simeq 10$ and $Re \simeq 5795$) (center) and the ideal case ($We \simeq 2.5$ and $Re \simeq 5795$) (bottom). In black, surfaces with an IRQ less than 2.

On Figure 3 (top), the unability of DNS to describe the original case is shown. The majority of the droplets present a low IRQ and, consequently, are poorly represented. Moreover, the surface of the central jet is very wrinkled, presenting areas with high curvature which are not well resolved. The under-resolved regions represent, in this case, 33.5% of the surface ($IRQ < 1$ in Figure 4) and 26% of the surface is midly resolved ($1 < IRQ < 2$ in Figure 4). The averaged in time PDF (Probability Density Function) of IRQ (Figure 5 top left) confirms the previous observation with a peak around an IRQ value of 0.6 and a low standard deviation. The PDF tends rapidly toward 0 for low values of IRQ. As expected, we can see that for this particular range of high Weber and Reynolds numbers, performing an

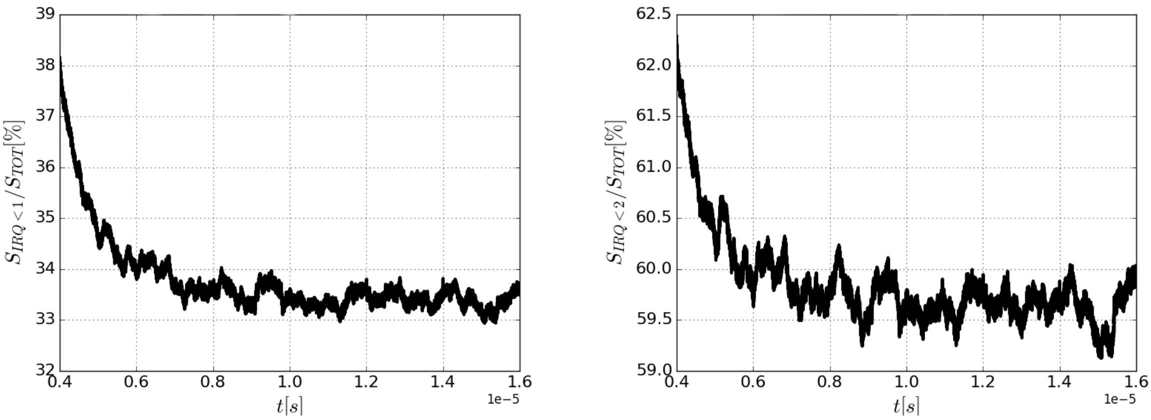

Figure 4. Temporal evolution of the percentage of surface with an IRQ less than 1 (left) and less than 2 (right) for the original Spray A configuration ($We \simeq 1044$ and $Re \simeq 70356$).

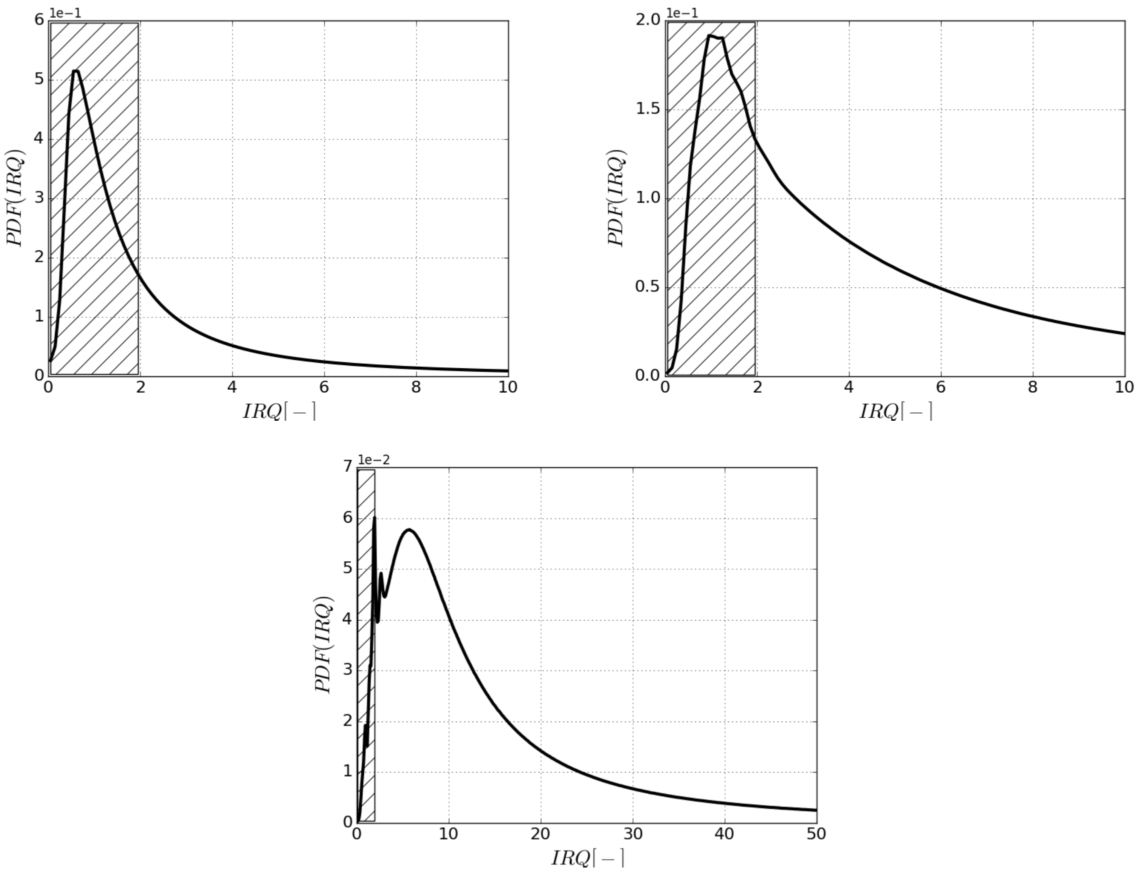

Figure 5. PDF of IRQ averaged in time for the original ($We \simeq 1044$ and $Re \simeq 70356$) (top left), the low Weber and Reynolds numbers ($We \simeq 10$ and $Re \simeq 5795$) (top right) and the ideal ($We \simeq 2.5$ and $Re \simeq 5795$) (bottom) Spray A configuration. The hatched part corresponds to the under-resolved zone ($IRQ < 2$).

accurate computation is a challenging task.

Most simulations of jet are performed with lower Weber and Reynolds numbers. This kind of simulation is represented on Figure 3 (center). In this case, the majority of the under-resolved surfaces comes from the little droplets at the periphery of the central jet. However, here, much less black regions are visible. Due to the low level of turbulence (low Reynolds number) and the high surface tension force (low Weber number), all the instabilities with a high frequency are damped and the developed structures have a lower curvature allowing a better resolution. The percentage of surface midly resolved is somewhat lower than the original case but the under-resolved surfaces are strongly reduced (Figure 6). It corresponds to only 8% of the total surface. The PDF of IRQ (Figure 5 top right) is shifted toward the higher values of IRQ and the peak is around 1.1. Higher values of IRQ and, so, lower values of curvature are more represented and the PDF profile is more smeared than the previous case. Even if this case with lower Weber and Reynolds numbers is obviously more resolved than the original case, there is still 23% of the surface that has an IRQ less than 2, illustrating an accuracy not as good as expected. However, it's more difficult to be well resolved in this kind of simulation where the injected turbulence have wider ranges of scales, which are consequently atomizing more the jet, than other studies with similar parameters but where the synthetic injected turbulence is mostly composed of large scales (see [3] for instance).

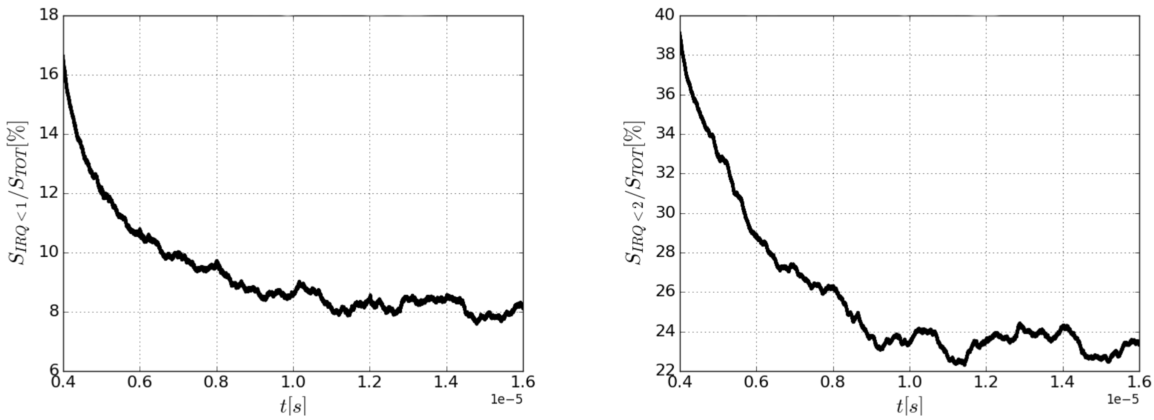

Figure 6. Temporal evolution of the percentage of surface with an IRQ less than 1 (left) and less than 2 (right) for the low Weber and Reynolds numbers Spray A configuration ($We \simeq 10$ and $Re \simeq 5795$).

Table 4. Physical parameters for the ideal ECN Spray A configuration.

ρ_g $(kg \cdot m^{-3})$	ρ_l $(kg \cdot m^{-3})$	μ_g $(kg \cdot m^{-1} \cdot s^{-1})$	μ_l $(kg \cdot m^{-1} \cdot s^{-1})$	σ $N \cdot m^{-1}$
22.8	713	1.8343×10^{-5}	8.8×10^{-3}	10.16

Finally, in order to see what parameters have to be chosen to have an accurate simulation of the jet, a third case with this time $We \simeq 2.5$ and $Re \simeq 5795$ has been performed. The parameters are reported on Table 4.

Only a small fraction of the total surface is now under-resolved (Figure 3 bottom). Even if the simulation is much longer to reach a steady state (Figure 7), results obtained show that the mean percentage of surface that has an IRQ less than 2 is around 2% and only 0.4% of the surface is really under-resolved ($IRQ < 1$). Also, the peak of the PDF of IRQ is now in the resolved part of the graph and is around an IRQ value of 6 (Figure 5 bottom). This third case is obviously well resolved but to reach this level of accuracy, unrealistic physical parameters have to be chosen and the jet atomizes itself with a few production of droplets.

Regarding the original Spray A case with high Weber and Reynolds numbers, even if the level of accuracy is low, a satisfying agreement with the experiment [19] can nevertheless be obtained. Indeed, the mean liquid volume fraction profile (Figure 8) is well captured at the center but is under estimated at the periphery, showing that the big scales are well represented whereas the little ones are less captured.

Conclusions

An estimation of a new surface resolution criterion called IRQ is performed in this work and used in two main configurations: the Spray A liquid jet from ECN and the two-phase homogenous isotropic turbulence. The HIT configuration serves as a reference to see the accuracy that can be expected on a well-resolved case. On this case, it is shown that, even for a well resolved case, there are always under-resolved regions like in breakup events which can not be captured. Then, the Spray A configuration points out the fact that a good resolution is difficult to reach for realistic parameters and low Weber and Reynolds numbers are required to capture the main flow characteristics. Results from the HIT and more quantitative statistics based on this criterion will be presented at the conference to illustrate the potential of the criterion.

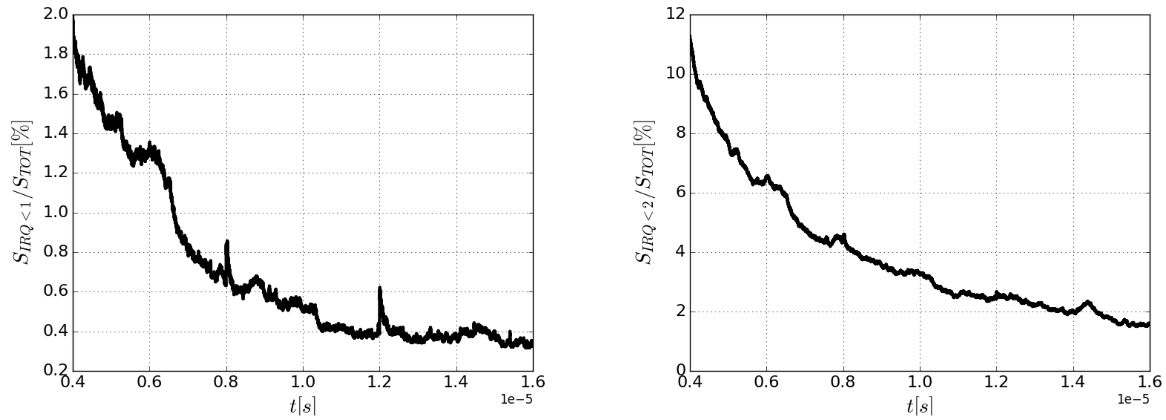

Figure 7. Temporal evolution of the percentage of surface with an IRQ less than 1 (left) and less than 2 (right) for the ideal Weber and Reynolds numbers Spray A configuration ($We \simeq 2.5$ and $Re \simeq 5795$).

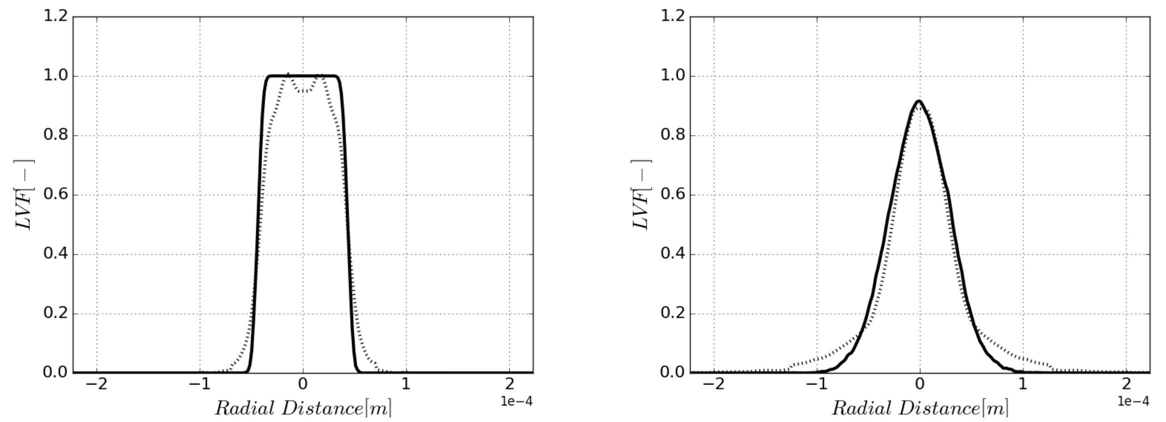

Figure 8. Mean liquid volume fraction radial profiles at $1.1\ D_{inj}$ (left) and $19\ D_{inj}$ (right) for the original Spray A configuration ($We \simeq 1044$ and $Re \simeq 70356$). DNS results are shown in solid line and ECN experiment, in dotted line.

Acknowledgements
The presented work was performed using computing resources of CRIANN (Normandy, France). This work was granted access to the HPC resources of IDRIS, TGCC and CINES under the allocations A0032B10101 and A0052B10101 made by GENCI (Grand Equipement National de Calcul Intensif).

Nomenclature

P	Pressure $[Pa]$
$\vec{u}$	Velocity vector $[m \cdot s^{-1}]$
ρ	Density $[kg \cdot m^{-3}]$
μ	Dynamic viscosity $[kg \cdot m^{-1} \cdot s^{-1}]$
σ	Surface tension $[N \cdot m^{-1}]$
φ	Distance from the interface $[m]$
Σ	Mean surface density $[m^{-1}]$
κ_1, κ_2	Main curvatures $[m^{-1}]$
k_{kin}	Turbulent kinetic energy $[m^2 \cdot s^{-2}]$
τ_t	Turbulent time $[-]$

Acronyms

CLSVOF	Coupled Level Set Volume Of Fluid
DNS	Direct Numerical Simulation
ECN	Engine Combustion Network
ELSA	Eulerian Lagrangian Spray Atomization
GF	Ghost Fluid
HIT	Homogeneous Isotropic Turbulence

IRQ Interface Resolution Quality
LES Large Eddy Simulation
PDF Probability Density Function
VOF Volume Of Fluid

References

[1] Olivier Desjardins, Vincent Moureau, and Heinz Pitsch. An accurate conservative level set/ghost fluid method for simulating turbulent atomization. *Journal of Computational Physics*, 227(18):8395–8416, September 2008.

[2] M. Herrmann. A balanced force refined level set grid method for two-phase flows on unstructured flow solver grids. *Journal of Computational Physics*, 227(4):2674–2706, February 2008.

[3] T. Ménard, S. Tanguy, and A. Berlemont. Coupling level set/VOF/ghost fluid methods: Validation and application to 3d simulation of the primary break-up of a liquid jet. *International Journal of Multiphase Flow*, 33(5):510–524, May 2007.

[4] Mikhael Gorokhovski and Marcus Herrmann. Modeling Primary Atomization. *Annual Review of Fluid Mechanics*, 40(1):343–366, 2008.

[5] J. Shinjo and A. Umemura. Simulation of liquid jet primary breakup: Dynamics of ligament and droplet formation. *International Journal of Multiphase Flow*, 36(7):513–532, July 2010.

[6] J. Anez, A. Ahmed, N. Hecht, B. Duret, J. Reveillon, and F. X. Demoulin. Eulerian–Lagrangian spray atomization model coupled with interface capturing method for diesel injectors. *International Journal of Multiphase Flow*, October 2018.

[7] R. Lebas, T. Menard, P. A. Beau, A. Berlemont, and F. X. Demoulin. Numerical simulation of primary break-up and atomization: DNS and modelling study. *International Journal of Multiphase Flow*, 35(3):247–260, March 2009.

[8] Ariane Vallet and Roland Borghi. Modélisation eulerienne de l'atomisation d'un jet liquide. *Comptes Rendus de l'Académie des Sciences-Series IIB-Mechanics-Physics-Astronomy*, 327(10):1015–1020, 1999.

[9] Romain Canu, Stefano Puggelli, Mohamed Essadki, Benjamin Duret, Thibaut Menard, Marc Massot, Julien Reveillon, and F. X. Demoulin. Where does the droplet size distribution come from? *International Journal of Multiphase Flow*, 107:230–245, October 2018.

[10] B. Duret, J. Reveillon, T. Menard, and F. X. Demoulin. Improving primary atomization modeling through DNS of two-phase flows. *International Journal of Multiphase Flow*, 55:130–137, October 2013.

[11] G. Vaudor, T. Ménard, W. Aniszewski, M. Doring, and A. Berlemont. A consistent mass and momentum flux computation method for two phase flows. Application to atomization process. *Computers & Fluids*, 152:204–216, July 2017.

[12] M. Sussman, K. M. Smith, M. Y. Hussaini, M. Ohta, and R. Zhi-Wei. A sharp interface method for incompressible two-phase flows. *Journal of Computational Physics*, 221(2):469–505, February 2007.

[13] M. Kang, R. P. Fedkiw, and X.D. Liu. Boundary conditions capturing method for multiphase incompressible flow. *Journal of Scientific Computing*, 3:323–360, 2000.

[14] Xu-Dong Liu, Ronald P. Fedkiw, and Myungjoo Kang. A Boundary Condition Capturing Method for Poisson's Equation on Irregular Domains. *Journal of Computational Physics*, 160(1):151 – 178, 2000.

[15] Gordon Kindlmann, Ross Whitaker, Tolga Tasdizen, and Torsten Moller. Curvature-based transfer functions for direct volume rendering: Methods and applications. In *Visualization, 2003. VIS 2003. IEEE*, pages 513–520. IEEE, 2003.

[16] B. Duret, G. Luret, J. Reveillon, T. Menard, A. Berlemont, and F. X. Demoulin. DNS analysis of turbulent mixing in two-phase flows. *International Journal of Multiphase Flow*, 40:93–105, April 2012.

[17] B Duret, T Menard, J Reveillon, and F X Demoulin. A DNS database to improve atomization modeling. page 7, 2012.

[18] Zakaria Bouali, Benjamin Duret, François-Xavier Demoulin, and Arnaud Mura. DNS analysis of small-scale turbulence-scalar interactions in evaporating two-phase flows. *International Journal of Multiphase Flow*, 85:326–335, October 2016.

[19] Engine Combustion Network | Near-nozzle mixture derived from x-ray radiography. `https://ecn.sandia.gov/rad675/`.